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Alloy element induced vacancy clustering in W-Re/Ta material

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Alloying elements can possibly serve as an important technique in designing W-based plasma facing materials (PFMs) with superior comprehensive performance. To investigate the interaction between the alloying elements and point defect is one of the mainly contents to study the W material service properties under irradiation. The first-principle method based on the density function theory was used to investigate the laws for the movements of the point defects in case of the alloying metal Re/Ta solution atoms. It was found from the formation energy and binding energy that Rhenium would be a potent factor to form the mono-vacancy than Ta in W alloying system. The mono-vacancy diffusion in W-Re/Ta alloy was studied via the pathways models, in which Re atom can steady exist in tungsten lattice while Ta solute atom was beneficial to move to a vacancy. Although the replacement atoms were different, it could find that both solute Re and Ta atoms manifest the positive effects to mono-vacancy migration in irradiation environment. According the average relaxed volume, the attraction interaction of vacancy cluster can be interpreted rationally. The important thing was that Re contributed the vacancy to form clusters configuration, but Ta had an inhibiting effect on diminutive vacancy cluster (n≤3), and it can be furthered concluded that Ta could control the point defects from gathering together, especially when its concentration was enlarged. These results can be used to construct the design basis of the W-based alloying in terms of improving the radiation resistance in the fusion environment.

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